Supporting Information

Novel Energetic Metal-organic Frameworks Assembled with the Energetic Combination of Furazan and Tetrazole

Hao, Wenjia[a]; Jin, Bo[a*]; Zhang, Jinhao[a]; Li, Xiaoyi[a]; Huang, Tao[a]; Shen, Juan[b]; Peng, Rufang[a]

a State Key Laboratory of Environment-friendly Energy Materials, Southwest University of Science and Technology, Sichuan Mianyang 621010, China

b School of Materials Science and Engineering, Southwest University of Science and Technology, Mianyang 621010, China

* jinbo0428@163.com

1. Instruments and reagents

The FT-IR spectra were recorded on a *PerkinElmer Spectrum 100* infrared spectrometer (KBr pellets) in the range of 4000 – 400 cm^{-1} with a resolution of 4 cm^{-1}. Elemental analyses of C, H and N were performed on a Vario EL-III analyzer. TGA-DSC measurement was carried by using *404 F1* differential scanning calorimeter (*Netzsch*).

2. FT-IR

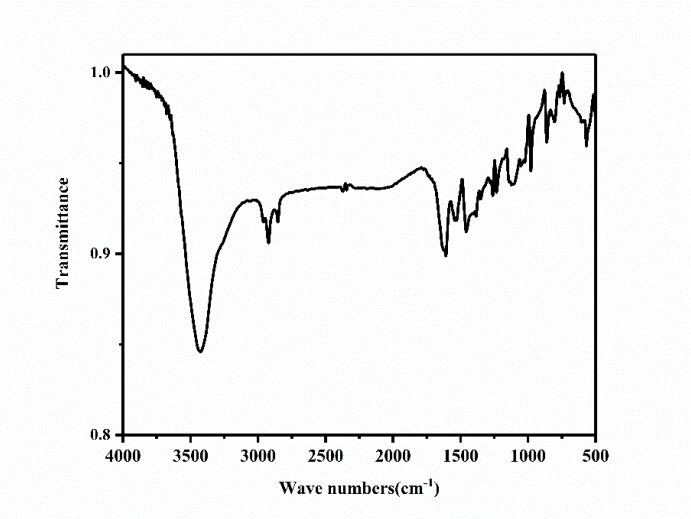

Figure S1. FT-IR spectrum of $[Pb(BTF)(H_2O)_2]_n$

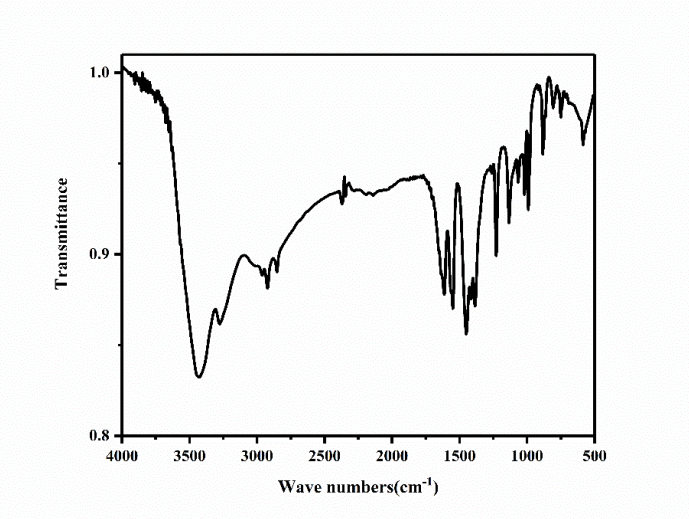

Figure S2. FT-IR spectrum of $[Ba(BTF)(H_2O)_4]_n$

3. X-ray crystallographic data

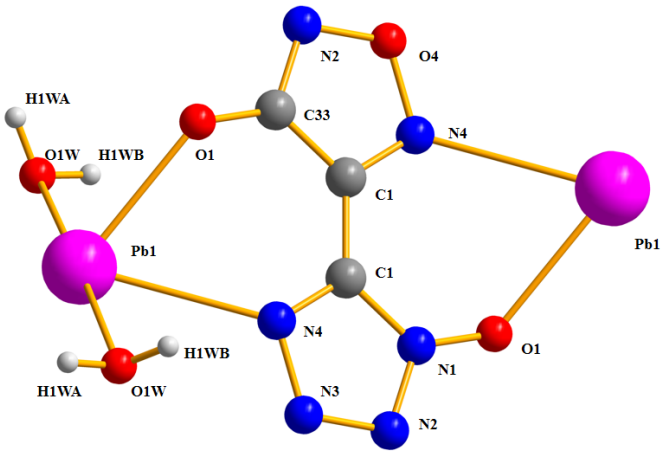

Figure S3. Coordination environment of Pb(II).

Table S1. Bond Lengths [Å] for $[Pb(BTF)(H_2O)_2]_n$

Bond	**Length/Å**
Pb1-O1[1]	2.593(3)
Pb1-O1	2.605(3)
Pb1-O1[2]	2.593(3)
Pb1-N4	2.845(2)
Pb1-O1[3]	2.605(3)
Pb1-O1W[3]	2.648(4)
Pb1-O1W	2.648(4)
O1-Pb1[4]	2.593(3)
O1-N1	1.306(6)
O1-C3	1.306(6)

N1-N2	1.329(6)
N1-C1	1.397(6)
N2-N3	1.363(5)
N2-C3	1.329(6)
N2-O4	1.363(5)
N3-N4	1.366(5)
N4-C1	1.317(6)
N4-O4	1.366(5)
C1-C1[5]	1.499(8)
C1-C3[3]	1.397(6)
[1]1-X,-1+Y,1/2-Z; [2]+X,-1+Y,+Z; [3]1-X,+Y,1/2-Z; [4]+X,1+Y,+Z; [5]1-X,1-Y,1-Z	

Table S2. Bond Angles [°] for $[Pb(BTF)(H_2O)_2]_n$.

Bond	**Angle/**°	**Bond**	**Angle/**°
O1[1]-Pb1-O1[2]	64.30(16)	C33-O1-Pb1[4]	114.6(2)
O1[2]-Pb1-O1	115.86(15)	C33-O1-Pb1	128.7(2)
O11-Pb1-O1	179.84(6)	O1-N1-N2	123.1(4)
O1[1]-Pb1-O1[3]	115.86(15)	O1-N1-C1	128.4(4)
O1[2]-Pb1-O1[3]	179.84(6)	N2-N1-C1	108.4(4)
O1[3]Pb1-O1	63.98(16)	N2-N3-N4	111.0(3)
O1-Pb1-O1W[3]	76.19(12)	C1-N4-N3	105.7(4)
O1[2]-Pb1-O1W[3]	73.89(12)	C1-N4-O4	105.7(4)
O1[1]-Pb1-O1W[3]	103.88(12)	N1-C1-C1[5]	126.0(5)
O1[2]-Pb1-O1W	103.88(12)	N4-C1-N1	109.2(4)
O1[3]-Pb1-O1W[3]	106.04(12)	N4-C1-C1[5]	124.8(5)
O1-Pb1-O1W	106.04(12)	N4-C1-C33	109.2(4)
O1[1]-Pb1-O1W	73.89(12)	C33-C1-C1[5]	126.0(5)
O1[3]-Pb1-O1W	76.19(12)	O1-C33-N2	123.1(4)
O1W-Pb1-O1W[3]	177.45(15)	O1-C33-C1	128.4(4)
Pb1[4]-O1-Pb1	115.86(15)	N2-C33-C1	108.4(4)
N1-O1-Pb1[4]	114.6(2)	N2-O4-N4	111.0(3)
N1-O1-Pb1	128.7(2)		
[1]1-X,-1+Y,1/2-Z; [2]+X,-1+Y,+Z; [3]1-X,+Y,1/2-Z; [4]+X,1+Y,+Z; [5]1-X,1-Y,1-Z			

Table S3. Hydrogen Bond Lengths and Bond Angles for $[Pb(BTF)(H_2O)_2]_n$ [[Å] and [°]].

Bond D-H···A	**Length/Å** (D-H)	**Length/Å** (H···A)	**Length/Å** (D···A)	**Angle/**° (DHA)
O(1W)-H(1WB)···O(1W)[6]	0.87(2)	1.86(3)	2.710(5)	168(7)
O(1W)-H(1WA)···N(2)[1]	0.86(2)	2.36(5)	3.003(5)	131(6)
O(1W)-H(1WA)···N(3^c)[7]	0.86(2)	2.40(5)	3.022(5)	130(5)
[1]-x+1/2,y+1/2,-z+1/2;[2] -x+1,y-1,-z+1/2;[3] x-1/2,-y+3/2,z-1/2				

Table S4. Atomic Occupancy for $[Pb(BTF)(H_2O)_2]_n$.

Atom	Occupancy	Atom	Occupancy
N1	0.5	N3	0.5
O4	0.5	C33	0.5

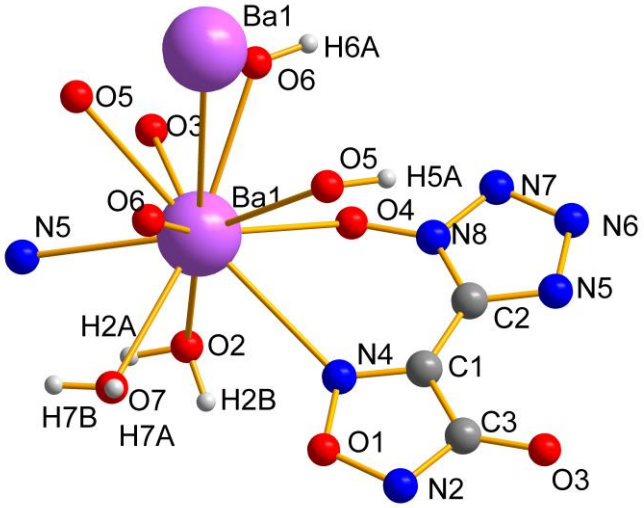

Figure S4. Coordination environment of Ba(II).

Table S5. Bond Lengths [Å] for $[Ba(BTF)(H_2O)_4]_n$

Bond	Length/Å
Ba1-O4	2.724(5)
Ba1-O2	2.764(6)
Ba1-O3^1	2.767(5)
Ba1-O6	2.793(5)
Ba1-O6^2	2.830(6)
Ba1-O7	2.910(6)
Ba1-N5^1	2.953(6)
Ba1-O5	2.961(5)
Ba1-O5^2	3.000(5)
Ba1-N4	3.109(6)
Ba1-Ba1^2	4.1958(8)
O1-N4	1.368(8)
O1-N2	1.381(8)
C1-N4	1.312(10)
C1-C3	1.411(10)
C1-C2	1.452(10)
O2-H2A	0.9269
O2-H2B	0.9276
C2-N5	1.332(10)
C2-N8	1.363(10)

N2-C3	1.326(9)
O3-C3	1.291(9)
O4-N8	1.302(8)
N5-N6	1.360(8)
O5-H5A	0.95
N6-N7	1.342(9)
O6-H6A	0.95
N7-N8	1.329(9)
O7-H7A	0.907
O7-H7B	0.9067
[1]-x+3/2,y+1/2,-z+3/2 [2] -x+1,-y+1,-z+2 [3] -x+3/2,y-1/2,-z+3/2	

Table S6. Bond Angles [°] for $[Ba(BTF)(H_2O)_4]_n$ **.**

Bond	**Angle/°**	**Bond**	**Angle/°**
O4-Ba1-O2	72.84(18)	O2-Ba1-Ba1[2]	175.49(13)
O4-Ba1-O3[1]	78.54(16)	O3[1]-Ba1-Ba1[2]	100.87(12)
O2-Ba1-O3[1]	74.92(18)	O6-Ba1-Ba1[2]	42.07(11)
O4-Ba1-O6	75.11(16)	O6[2]-Ba1-Ba1[2]	41.40(11)
O2-Ba1-O6	135.68(18)	O7-Ba1-Ba1[2]	106.90(14)
O3[1]-Ba1-O6	69.32(16)	N5[1]-Ba1-Ba1[2]	112.01(12)
O4-Ba1-O6[1]	135.71(16)	O5-Ba1-Ba1[2]	45.64(10)
O2-Ba1-O6[1]	140.53(17)	O5[2]-Ba1-Ba1[2]	44.88(10)
O3[1]-Ba1-O6[1]	128.91(16)	N4-Ba1-Ba1[2]	111.26(13)
O6-Ba1-O6[2]	83.47(17)	N4-O1-N2	110.9(5)
O4-Ba1-O7	128.98(17)	N4-C1-C3	109.6(6)
O2-Ba1-O7	75.08(19)	N4-C1-C2	124.3(7)
O3[1]-Ba1-O7	128.64(19)	C3-C1-C2	126.1(7)
O6-Ba1-O7	148.92(18)	Ba1-O2-H2A	111.4
O62-Ba1-O7	65.53(18)	Ba1-O2-H2B	111.9
O4-Ba1-N5[1]	127.85(18)	H2A-O2-H2B	102.3
O2-Ba1-N5[1]	64.77(18)	N5-C2-N8	109.0(6)
O3[1]-Ba1-N5[1]	62.57(16)	N5-C2-C1	124.0(7)
O6-Ba1-N5[1]	116.78(16)	N8-C2-C1	127.0(7)
O6[2]-Ba1-N5[1]	96.38(16)	C3-N2-O1	105.6(6)
O7-Ba1-N5[1]	67.16(19)	C3-O3-Ba1[3]	140.0(5)
O4-Ba1-O5	76.46(16)	O3-C3-N2	123.4(7)
O2-Ba1-O5	138.24(16)	O3-C3-C1	128.5(7)
O3[1]-Ba1-O5	125.45(15)	N2-C3-C1	108.1(6)
O6-Ba1-O5	57.72(14)	N8-O4-Ba1	136.4(5)
O6[2]-Ba1-O5	59.37(14)	C1-N4-O1	105.7(6)
O7-Ba1-O5	104.57(18)	C1-N4-Ba1	128.2(5)
N5[1]-Ba1-O5	154.73(16)	O1-N4-Ba1	122.0(4)
O4-Ba1-O52	131.84(15)	C2-N5-N6	105.7(6)

O2-Ba1-O52	131.15(16)	C2-N5-Ba1[3]	135.4(5)
O31-Ba1-O52	72.02(16)	N6-N5-Ba1[3]	117.2(4)
O6-Ba1-O52	59.27(14)	Ba1-O5-Ba1[2]	89.48(14)
O6[2]-Ba1-O52	56.89(14)	Ba1-O5-H5A	119.8
O7-Ba1-O52	99.11(16)	Ba1[2]-O5-H5A	126.7
N5[1]-Ba1-O52	68.38(16)	N7-N6-N5	110.2(6)
O5-Ba1-O52	90.52(14)	Ba1-O6-Ba1[2]	96.53(17)
O4-Ba1-N4	60.90(16)	Ba1-O6-H6A	119.9
O2-Ba1-N4	73.14(18)	Ba1[2]-O6-H6A	127.7
O3[1]-Ba1-N4	133.97(17)	N8-N7-N6	106.7(6)
O6-Ba1-N4	115.49(16)	Ba1-O7-H7A	111
O6[2]-Ba1-N4	96.48(16)	Ba1-O7-H7B	110.6
O7-Ba1-N4	72.43(18)	H7A-O7-H7B	103.2
N5[1]-Ba1-N4	127.17(17)	O4-N8-N7	122.8(6)
O5-Ba1-N4	67.39(16)	O4-N8-C2	128.8(7)
O52-Ba1-N4	152.45(16)	N7-N8-C2	108.4(6)
[1]-x+3/2,y+1/2,-z+3/2 [2] -x+1,-y+1,-z+2 [3] -x+3/2,y-1/2,-z+3/2			

Table S7. Hydrogen bonds for $[Ba(BTF)(H_2O)_4]_n$ [Å and °].

Bond D-H···A	**Length/Å** (D-H)	**Length/Å** (H···A)	**Length/Å** (D···A)	**Angle/**° (DHA)
O(2)-H(2A)···O(1)[1]	0.93	2.18	3.005(8)	147.6
O(2)-H(2A)···N(5)[2]	0.93	2.59	3.067(8)	112.5
O(2)-H(2B)···O(7)[1]	0.93	2.04	2.795(8)	137.4
O(5)-H(5A)···N(2)[3]	0.95	2.05	2.910(8)	149.8
O(6)-H(6A)···O(3)[3]	0.95	1.79	2.699(7)	160
O(7)-H(7A)···O(2)[4]	0.91	2.51	3.071(9)	120.2
O(7)-H(7A)···O(4)[4]	0.91	2.36	3.193(9)	152.8
O(7)-H(7B)···N(6)[2]	0.91	2.15	2.872(10)	136.4
[1] -x+1,-y+1,-z+1 [2] -x+3/2,y+1/2,-z+3/2 [3] x+1/2,-y+1/2,z+1/2 [4] x-1,y,z				